

REMARKS/ARGUMENTS

Claims Objections

The Examiner has noted that periods were used after step letter indicators so that there were a "multiplicity of periods" in the claims rather than one at the end. Correction has been made by the substitution of a parentheses for the period after each step letter indicator.

Claim Rejections - 35 U.S.C § 112 second paragraph

The Examiner has rejected: "...claims 1-7, step 2a in each, the use of parenthetical expressions renders the claim indefinite because it is unclear whether the limitation(s) in the parentheses are part of the claimed invention." Applicants do not understand why the Examiner might assume that any language appearing in the claim, whether set off by parentheses or not, would not be considered part of the claim. Applicants intend the material within the parentheses to be part of the claim. Applicants have amended the claims to set off the same material with commas, but Applicants believe that the material is part of the claims whether set off by parentheses or by commas.

Additional Claim Rejections

The Examiner has rejected the claims on the following bases:

35 U.S.C § 112 first paragraph

- new rejection - claims fail to comply with the written description requirement
- new rejection - claimed invention is not supported by specific, substantial or credible asserted utility

35 U.S.C § 112 second paragraph

- new rejection - claims are indefinite for failing to particularly point out and distinctly claim the subject matter

35 U.S.C. § 101

- claimed invention is directed to non-statutory subject matter

While the Examiner has characterized each rejection in accordance with the standards of the statutory section under which the rejection is based, there is a common thread that runs through and underlies all the rejections. Specifically, what appears to Applicants to be the problem is that the Examiner believes that, since there are no actual molecules described or molecular structures produced by the implemented processes, nothing substantive or useful is taught. Applicants respectfully disagree with the Examiner. What is taught in the patent and set forth in the claims are molecules which can be selected by a highly specific process from a vast universe of possible molecules which selected molecules share a specific useful characteristic. In particular, since molecular structural descriptors possessing a neighborhood property are used in the process of selection, the molecules which are selected will all possess similar three dimensional shape characteristics which suggest that they will have a higher likelihood of possessing similar biological activity.

Applicants have amended the claims to more specifically characterize this useful feature of the invention and believe that with the amendments the problems cited by the Examiner under each basis of rejection are eliminated. The major amendments have been made to the claim preambles, and Applicants intend that the preambles be read as an integral part of the claims with the limitations recited in the preamble.

Applicants do not believe that claims directed to molecules having desired features in common must recite the specific molecular structures or families as long as it recites the specific method of identifying the molecules.

A user of the methods described in claims 1-4 will select a molecule in which he/she is interested and which can be constructed from the information in the virtual library. The result of the use of the methods will result in a group of molecules (having similar three dimensional shapes and highly likely similar biological activities) which sample the molecular shape space which can be achieved using many different structural variations (reagents), cores, and chemistries. The group will not be oversampled. Applicants would point out that the use of the validated descriptors places a limitation on the claimed molecules which are not known or anticipated by the prior art including Agrafiotis.

Claims 5-7 identify molecules likely to have the same activity as a specific molecule known to the user. The claimed molecules will have similar shape (as characterized by the validated molecular structural descriptors possessing a neighborhood property) and likely biological activity out of all the possible molecules which could be formed from the structural variations, cores, and chemistries in the virtual library. Again, the identified molecules will not be oversampled.

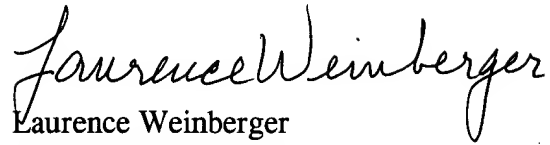
Applicants respectfully submit that a person reasonably skilled in the art of computational chemistry will know how to use the invention to achieve the selection results for the specific molecules that person is interested in. Accordingly, Applicants respectfully request that the Examiner remove the rejections of record and that a timely Notice of Allowance be issued in this

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Respectfully submitted,

A handwritten signature in cursive script that reads "Laurence Weinberger". The signature is written in black ink and is positioned above the printed contact information.

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